

Photoemission spectroscopy and sum rules in dilute electron-phonon systems

P. E. Kornilovitch

Hewlett-Packard Laboratories, MS 1L-12, 1501 Page Mill Road, Palo Alto, California, 94304
(February 1, 2008)

A family of exact sum rules for the one-polaron spectral function in the low-density limit is derived. An algorithm to calculate energy moments of arbitrary order of the spectral function is presented. Explicit expressions are given for the first two moments of a model with general electron-phonon interaction, and for the first four moments of the Holstein polaron. The sum rules are linked to experiments on momentum-resolved photoemission spectroscopy. The bare electronic dispersion and the electron-phonon coupling constant can be extracted from the first and second moments of spectrum. The sum rules could serve as constraints in analytical and numerical studies of electron-phonon models.

PACS numbers: 71.38.-k, 79.60.-i

Statistical analysis of spectra is an important branch of photoemission spectroscopy. It has been known that the energy moments of the spectral density of atoms can be expressed via the atomic quantum numbers [1,2]. Such integral relations, or sum rules, provide direct link between experimental data and the internal state of the atoms. Similarly, in crystals analogous sum rules yield valuable information about the Bloch states. This is particularly true in case of two-dimensional systems where the in-plane momentum of the electron does not change in the photoemission process. It allows the spectrum to be recorded for each in-plane momentum individually. In recent years, the angle-resolved photoemission spectroscopy became a powerful experimental technique to study the electronic structure of quasi-two-dimensional compounds such as the high-temperature superconductors and layered colossal magnetoresistive oxides [3–5].

This paper discusses statistical analysis of spectra from systems with strong electron-phonon (el-ph) interaction. In such systems, the mobile carriers deform the lattice and form polarons which are bound states of the carriers and the lattice deformations. The polarons then define the low-energy physics of the system, in particular the equilibrium chemical potential. In inverse photoemission (IPES), an electron with momentum \mathbf{k} is injected into the system from outside. Initially it feels the bare electronic states in the undeformed lattice and only then begins to deform the lattice around itself. Thus it should be expected that the energy moments of the IPES intensity could provide information about the initial stages of the deformation process and therefore about the strength of the interaction. It turns out that for low density of polarons the moments of IPES intensity can be calculated analytically for a wide class of model el-ph interactions. It leads to a series of exact sum rules which the spectral density, experimental or theoretical, must satisfy. Below I derive the sum rules and discuss their possible applications.

Consider a single band, one optical branch Hamiltonian with an el-ph interaction of arbitrary profile [6,7]

$$\mathcal{H} = \sum_{\mathbf{k}} (\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}}^\dagger c_{\mathbf{k}} - \sqrt{2\Omega} \sum_{\mathbf{nm}} g(\mathbf{n} - \mathbf{m}) c_{\mathbf{n}}^\dagger c_{\mathbf{n}} x_{\mathbf{m}} + \frac{\Omega}{2} \sum_{\mathbf{m}} (-\partial_{\mathbf{m}}^2 + x_{\mathbf{m}}^2). \quad (1)$$

Here μ is the chemical potential, $x_{\mathbf{m}} = \xi_{\mathbf{m}} \sqrt{\frac{M\Omega}{\hbar}}$ is the dimensionless displacement of an oscillator at \mathbf{m} -th lattice site, M and Ω are the mass and the frequency of the oscillators, respectively, $\partial_{\mathbf{m}} \equiv \partial/\partial x_{\mathbf{m}}$, $c_{\mathbf{n}} = N^{-1/2} \sum_{\mathbf{k}} e^{i\mathbf{kn}} c_{\mathbf{k}}$, and N is the number of lattice sites. $g(\mathbf{n} - \mathbf{m})$ is the dimensionless coupling constant proportional to the force with which an electron at site \mathbf{n} acts on oscillator \mathbf{m} . For simplicity, the fermion spin and multiple phonon polarizations are not included explicitly in Eq.(1). They are not essential for the purposes of the paper and could be added if necessary. The canonical Holstein model [8] follows from the above Hamiltonian with the choice $g(\mathbf{n} - \mathbf{m}) = g_0 \delta_{\mathbf{nm}}$.

Within the sudden approximation, direct and inverse photoemission intensities are proportional to the fermion spectral functions $A_-(\mathbf{k}, \omega)$ and $A_+(\mathbf{k}, \omega)$, respectively (hereafter notation $\hbar = 1$ is used):

$$A_-(\mathbf{k}, \omega) = \frac{2\pi}{Z} \sum_{ij} e^{-\beta\mathcal{E}_i} |\langle j|c_{\mathbf{k}}|i\rangle|^2 \delta(\omega + \mathcal{E}_j - \mathcal{E}_i), \quad (2)$$

$$A_+(\mathbf{k}, \omega) = \frac{2\pi}{Z} \sum_{ij} e^{-\beta\mathcal{E}_i} |\langle j|c_{\mathbf{k}}^\dagger|i\rangle|^2 \delta(\omega + \mathcal{E}_i - \mathcal{E}_j). \quad (3)$$

Here ω is the energy relative to the chemical potential, $|i\rangle$ and $|j\rangle$ are exact eigenstates of \mathcal{H} , with energies \mathcal{E}_i and \mathcal{E}_j , $Z = \sum_n e^{-\beta\mathcal{E}_i}$ is the grand canonical partition function, and $\beta = (k_B T)^{-1}$. The validity of the sudden approximation as well as the additional electron-photon

matrix element, the Coulomb effects and other complications, are not going to be discussed in this paper, see e.g. [9]. It follows from Eqs. (2) and (3) that the two spectral functions obey the fundamental relation

$$A_+(\mathbf{k}, \omega) = e^{\beta\omega} A_-(\mathbf{k}, \omega). \quad (4)$$

Thus, A_+ can be found if A_- is known with sufficient accuracy, and visa versa. In terms of the symmetrized function $A = A_+ + A_-$ they are expressed as $A_-(\mathbf{k}, \omega) = (e^{\beta\omega} + 1)^{-1} A(\mathbf{k}, \omega)$ and $A_+(\mathbf{k}, \omega) = (e^{-\beta\omega} + 1)^{-1} A(\mathbf{k}, \omega)$.

Several theoretical results for the polaron spectral function are available. The on-site version of the Holstein model ($\varepsilon_{\mathbf{k}} \equiv 0$) is exactly solvable, see e.g. Ref. [10]. For the Holstein model with non-zero kinetic energy the spectral function was calculated by Alexandrov and Ranninger in the Lang-Firsov approximation [11]. Later their result was generalized to the long-range interaction (1) by Alexandrov and Sricheewin [12]. For the more complex Jahn-Teller interaction the polaron spectral function was given by Perebeinos and Allen [13]. The spectral functions mentioned are approximate and all have the form of a sequence of delta-functions.

The formalism of statistical moments is best introduced via the time-dependent correlation functions $K_{\pm}(\mathbf{k}, t)$ that are Fourier transforms of $A_{\pm}(\mathbf{k}, \omega)$:

$$\begin{aligned} K_+(\mathbf{k}, t) &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} A_+(\mathbf{k}, \omega) \\ &= \frac{1}{Z} \sum_j e^{-\beta\varepsilon_j} \langle j | e^{i\mathcal{H}t} c_{\mathbf{k}} e^{-i\mathcal{H}t} c_{\mathbf{k}}^\dagger | j \rangle \\ &\equiv \langle e^{i\mathcal{H}t} c_{\mathbf{k}} e^{-i\mathcal{H}t} c_{\mathbf{k}}^\dagger \rangle, \end{aligned} \quad (5)$$

$$\begin{aligned} K_-(\mathbf{k}, t) &= \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega t} A_-(\mathbf{k}, \omega) \\ &= \frac{1}{Z} \sum_j e^{-\beta\varepsilon_j} \langle j | c_{\mathbf{k}}^\dagger e^{i\mathcal{H}t} c_{\mathbf{k}} e^{-i\mathcal{H}t} | j \rangle \\ &= \langle c_{\mathbf{k}}^\dagger e^{i\mathcal{H}t} c_{\mathbf{k}} e^{-i\mathcal{H}t} \rangle. \end{aligned} \quad (6)$$

Taking the m -th derivative with respect to time t and setting $t = 0$ one obtains

$$\begin{aligned} \mathcal{M}_m^+(\mathbf{k}) &\equiv \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega^m A_+(\mathbf{k}, \omega) \\ &= \underbrace{\langle [[c_{\mathbf{k}}, \mathcal{H}], \mathcal{H}] \dots, \mathcal{H} \rangle}_{m \text{ times}} c_{\mathbf{k}}^\dagger, \end{aligned} \quad (7)$$

$$\begin{aligned} \mathcal{M}_m^-(\mathbf{k}) &\equiv \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} \omega^m A_-(\mathbf{k}, \omega) \\ &= \langle c_{\mathbf{k}}^\dagger \underbrace{\langle [[c_{\mathbf{k}}, \mathcal{H}], \mathcal{H}] \dots, \mathcal{H} \rangle}_{m \text{ times}} \rangle. \end{aligned} \quad (8)$$

The moments of the symmetrized function $A(\mathbf{k}, \omega)$ are defined as $\mathcal{M}_m(\mathbf{k}) = \mathcal{M}_m^+(\mathbf{k}) + \mathcal{M}_m^-(\mathbf{k})$.

The simplest sum rule is the normalization property of $A(\mathbf{k}, \omega)$ which is common to any one-particle fermionic spectral function

$$\mathcal{M}_0(\mathbf{k}) = \langle c_{\mathbf{k}} c_{\mathbf{k}}^\dagger + c_{\mathbf{k}}^\dagger c_{\mathbf{k}} \rangle = 1. \quad (9)$$

The first moment of $A(\mathbf{k}, \omega)$ is given by

$$\begin{aligned} [c_{\mathbf{k}}, \mathcal{H}] &= (\varepsilon_{\mathbf{k}} - \mu) c_{\mathbf{k}} \\ &\quad - \frac{\sqrt{2}\Omega}{N} \sum_{\mathbf{n} \mathbf{m} \mathbf{k}'} e^{i(\mathbf{k}' - \mathbf{k})\mathbf{n}} g(\mathbf{n} - \mathbf{m}) x_{\mathbf{n}} c_{\mathbf{k}'}. \end{aligned} \quad (10)$$

$$\begin{aligned} \mathcal{M}_1(\mathbf{k}) &= \langle [c_{\mathbf{k}}, \mathcal{H}] c_{\mathbf{k}}^\dagger + c_{\mathbf{k}}^\dagger [c_{\mathbf{k}}, \mathcal{H}] \rangle \\ &= (\varepsilon_{\mathbf{k}} - \mu) - \frac{\sqrt{2}\Omega}{N} \sum_{\mathbf{n} \mathbf{m}} g(\mathbf{n} - \mathbf{m}) \langle x_{\mathbf{m}} \rangle. \end{aligned} \quad (11)$$

The mean displacement of the oscillators $\langle x_{\mathbf{m}} \rangle$ depends only on the total number of carriers in the systems $\langle n \rangle$, and can be calculated as follows. Write the displacement operator as $x_{\mathbf{m}} = \langle x_{\mathbf{m}} \rangle + y_{\mathbf{m}}$ and substitute in \mathcal{H} . Then minimization of the free energy $F = -\beta^{-1} \ln \langle e^{-\beta\mathcal{H}} \rangle$ with respect to $\langle x_{\mathbf{m}} \rangle$ yields

$$\begin{aligned} \langle x_{\mathbf{m}} \rangle &= -\langle y_{\mathbf{m}} \rangle + \sqrt{2} \sum_{\mathbf{n}} g(\mathbf{n} - \mathbf{m}) \langle c_{\mathbf{n}}^\dagger c_{\mathbf{n}} \rangle \\ &= \sqrt{2} \langle n \rangle \sum_{\mathbf{n}} g(\mathbf{n}), \end{aligned} \quad (12)$$

because $\langle y_{\mathbf{m}} \rangle = 0$ by definition, and the mean density $\langle c_{\mathbf{n}}^\dagger c_{\mathbf{n}} \rangle = \langle n \rangle$ does not depend on coordinate \mathbf{n} . Substitution in Eq. (11) results in:

$$\mathcal{M}_1(\mathbf{k}) = (\varepsilon_{\mathbf{k}} - \mu) - 2\Omega \langle n \rangle \left[\sum_{\mathbf{n}} g(\mathbf{n}) \right]^2. \quad (13)$$

This is an exact relation for the one-particle spectral function. It is a generalization of the sum rule derived by Mahan for the on-site polaron [10], and by Perebeinos and Allen for the Jahn-Teller polaron [13], to non-zero polaron density. The main feature of these results is that the mean value of the spectral function is not affected by interaction with phonons. This conclusion is non-trivial in view of significant changes of the spectral function itself, especially in the strong coupling regime. As follows from Eq. (13), in the many-body case the first moment $\mathcal{M}_1(\mathbf{k})$ acquires a correction that is linear in polaron density. Proceeding with the calculation one obtains for the second moment

$$\begin{aligned} [[c_{\mathbf{k}}, \mathcal{H}], \mathcal{H}] &= (\varepsilon_{\mathbf{k}}^2 - \mu) c_{\mathbf{k}} \\ &\quad - \frac{\sqrt{2}\Omega}{N} \sum_{\mathbf{k}' \mathbf{n} \mathbf{m}} e^{i(\mathbf{k}' - \mathbf{k})\mathbf{n}} g(\mathbf{n} - \mathbf{m}) \\ &\quad \times [(\varepsilon_{\mathbf{k}} + \varepsilon_{\mathbf{k}'} - 2\mu) x_{\mathbf{m}} + \Omega \partial_{\mathbf{m}}] c_{\mathbf{k}'} \\ &\quad + \frac{2\Omega^2}{N} \sum_{\mathbf{k}' \mathbf{n} \mathbf{m} \mathbf{m}'} e^{i(\mathbf{k}' - \mathbf{k})\mathbf{n}} g(\mathbf{n} - \mathbf{m}) \\ &\quad \times g(\mathbf{n} - \mathbf{m}') x_{\mathbf{m}} x_{\mathbf{m}'} c_{\mathbf{k}'}, \end{aligned} \quad (14)$$

$$\begin{aligned}
\mathcal{M}_2(\mathbf{k}) &= \langle [[c_{\mathbf{k}}, \mathcal{H}], \mathcal{H}]c_{\mathbf{k}}^\dagger + c_{\mathbf{k}}^\dagger [[c_{\mathbf{k}}, \mathcal{H}], \mathcal{H}] \rangle = (\varepsilon_{\mathbf{k}} - \mu)^2 \\
&\quad - \frac{\sqrt{2}\Omega}{N} \sum_{\mathbf{nm}} g(\mathbf{n} - \mathbf{m}) [2(\varepsilon_{\mathbf{k}} - \mu)\langle x_{\mathbf{m}} \rangle + \Omega \langle \partial_{\mathbf{m}} \rangle] \\
&\quad + \frac{2\Omega^2}{N} \sum_{\mathbf{nm'm'}} g(\mathbf{n} - \mathbf{m})g(\mathbf{n} - \mathbf{m}') \langle x_{\mathbf{m}} x_{\mathbf{m'}} \rangle. \quad (15)
\end{aligned}$$

Unfortunately, the mean values $\langle x_{\mathbf{m}} x_{\mathbf{m'}} \rangle$ cannot be calculated analytically which limits application of the last expression. In principle, such averages could be computed numerically by various techniques, rendering Eq. (15) a true sum rule. (It is worth noting in this respect that in the case of the Hubbard model, the first and second moments of the spectral function were calculated analytically by Nolting [14]. This finding enabled him to develop the moment approach to the Hubbard model.)

Further progress can be made by going to the low density limit $\langle n \rangle \ll 1$. It follows from definitions (2) and (3) that $A_- \propto \langle n \rangle$ while $A_+ \propto 1 - \langle n \rangle$. Therefore $\mathcal{M}_m^- \ll \mathcal{M}_m^+$ so that \mathcal{M}_m^- could be dropped from Eqs. (9), (11), and (15). More importantly, all the phonon operators can now be averaged easily. Indeed, in the low-density limit the lattice is largely undeformed. The function A_+ describes the process when an electron is created in an *empty* lattice and removed later. Thus whatever phonon operators appear as a result of multiple commutation with the Hamiltonian, they have to be averaged over the system of undeformed *independent* harmonic oscillators, which is always possible. For instance, the mean values entering Eq. (15) are $\langle x_{\mathbf{m}} \rangle = \langle \partial_{\mathbf{m}} \rangle = 0$, $\langle x_{\mathbf{m}} x_{\mathbf{m'}} \rangle = \frac{1}{2} \coth(\frac{1}{2}\beta\Omega) \delta_{\mathbf{mm'}}$. Collecting all the results one obtains the following sum rules for the spectral function $A_+(\mathbf{k}, \omega)$:

$$\mathcal{M}_0^+(\mathbf{k}) = 1 + \mathcal{O}(\langle n \rangle), \quad (16)$$

$$\mathcal{M}_1^+(\mathbf{k}) = (\varepsilon_{\mathbf{k}} - \mu) + \mathcal{O}(\langle n \rangle), \quad (17)$$

$$\begin{aligned}
\mathcal{M}_2^+(\mathbf{k}) &= (\varepsilon_{\mathbf{k}} - \mu)^2 \\
&\quad + \Omega^2 \coth(\frac{1}{2}\beta\Omega) \sum_{\mathbf{n}} g^2(\mathbf{n}) + \mathcal{O}(\langle n \rangle). \quad (18)
\end{aligned}$$

The above exact relations may be used for statistical analysis of inverse photoemission spectra (IPES) from low-density polaron systems. First of all, Eq. (16) allows proper normalization of the spectrum for each electron momentum \mathbf{k} . According to Eq. (17), the first moment yields the *bare* electronic spectrum inside the crystal. However, in an el-ph system the chemical potential μ is lowered by the polaron binding energy E_p . As a function of \mathbf{k} , $\mathcal{M}_1^+(\mathbf{k})$ never gets smaller than E_p . In other words, one should expect a gap of size E_p in IPES. The second moment $\mathcal{M}_2^+(\mathbf{k})$ also contains information about the strength of el-ph interaction. It is convenient to parameterize the latter in terms of the zero order (in hopping) binding energy of the polaron, $E_p^{(0)} \equiv \Omega \sum_{\mathbf{n}} g^2(\mathbf{n})$, see [7]. ($E_p^{(0)}$ is employed here as a shorthand notation only. It does not include the effects of the kinetic

energy and therefore it is not the true polaron energy, $E_p^{(0)} \neq E_p$.) The mean squared deviation of the spectrum, $\overline{(\Delta\omega)^2} = \mathcal{M}_2^+ - (\mathcal{M}_1^+)^2 = E_p^{(0)}\Omega \coth(\frac{1}{2}\beta\Omega)$, is a direct measure of $E_p^{(0)}$. It has to scale approximately linearly with the IPES gap. Notice, that $\overline{(\Delta\omega)^2} = E_p^{(0)}\Omega$ at low temperatures and $\overline{(\Delta\omega)^2} \approx 2E_p^{(0)}T$ at high temperatures T .

One should mention that sum rules on the function $A_-(\mathbf{k}, \omega)$ have also been discussed in relation to direct photoemission. In particular, Randeria et al introduced an approximate sum rule for the zeroth moment, $\mathcal{M}_0^- = n(\mathbf{k})$, where $n(\mathbf{k})$ is the mean occupation of the state \mathbf{k} [15]. This relation may not be generalizable to polaronic systems because in general $n(\mathbf{k})$ depends on the strength of the el-ph interaction and therefore is not known a priori.

Calculation of moments can be continued. The low density ensures that any fermionic operator that will arise after the multiple commutation of $c_{\mathbf{k}}$ with the Hamiltonian, will factor out. The remaining phonon operators may be complex but they will have to be averaged over the system of free phonons. Such an averaging can always be performed. The conclusion is that *any* moment of $A_+(\mathbf{k}, \omega)$ can in principle be calculated analytically. However, the algebra quickly becomes cumbersome. Therefore, I present only two more moments for the Holstein model with nearest neighbor hopping, i.e. for $g(\mathbf{n} - \mathbf{m}) = g_0 \delta_{\mathbf{nm}}$ and $\varepsilon_{\mathbf{k}} = -J \sum_{\mathbf{l}} e^{i\mathbf{kl}}$, \mathbf{l} numbering the nearest neighbors:

$$\mathcal{M}_3^+(\mathbf{k}) = (\varepsilon_{\mathbf{k}} - \mu)^3 + 2g_T^2\Omega^2(\varepsilon_{\mathbf{k}} - \mu) + g_0^2\Omega^3 + \mathcal{O}(\langle n \rangle), \quad (19)$$

$$\begin{aligned}
\mathcal{M}_4^+(\mathbf{k}) &= (\varepsilon_{\mathbf{k}} - \mu)^4 + g_T^2\Omega^2[3(\varepsilon_{\mathbf{k}} - \mu)^2 + zJ^2] \\
&\quad + 2g_0^2\Omega^3(\varepsilon_{\mathbf{k}} - \mu) + [g_T^2 + 3g_0^2]\Omega^4 + \mathcal{O}(\langle n \rangle), \quad (20)
\end{aligned}$$

where $g_T^2 \equiv g_0^2 \coth(\frac{1}{2}\beta\Omega)$, and z is the number of nearest neighbors in the lattice. In deriving $\mathcal{M}_3^+(\mathbf{k})$ and $\mathcal{M}_4^+(\mathbf{k})$ the following properties of the harmonic oscillator have been used: $\langle x_{\mathbf{m}} \partial_{\mathbf{m}} \rangle = -\frac{1}{2}$, and $\langle x_{\mathbf{m}}^4 \rangle = \frac{3}{4} \coth^2(\frac{1}{2}\beta\Omega)$. It is interesting that in the fourth moment the hopping integral J appears not only via the bare spectrum $\varepsilon_{\mathbf{k}}$ but also by itself. Thus $\mathcal{M}_4^+(\mathbf{k})$ is the first moment that explicitly distinguishes the dimensionality of the lattice through the number of nearest neighbors z . Apparently the higher order moments also distinguish different lattice topologies.

Apart from their relation to photoemission spectroscopy the sum rules may find more “theoretical” applications. First of all, they are valid for the single polaron which continues to draw theoretical interest. Formal transition in the above expressions to the canonical ensemble with one particle is done by setting $\mu = 0$. Thus

the sum rules could be useful checks for polaron spectral functions computed numerically by exact diagonalization [16], density matrix renormalization group [17], quantum Monte Carlo [18], or any other method. Secondly, the sum rules may provide information on the dynamics of polaron formation. For instance, the quantity $P_+(\mathbf{k}, t) = |K_+(\mathbf{k}, t)|^2$ is the probability that the phonon system remains unchanged after time t under the disturbance of an electron with momentum \mathbf{k} . On the other hand, $P_+(\mathbf{k}, t) = 1 - [\mathcal{M}_2^+(\mathbf{k}) - \mathcal{M}_1^{+2}(\mathbf{k})]t^2 + o(t^2) = 1 - E_p^{(0)}\Omega \coth(\frac{1}{2}\beta\Omega)t^2 + o(t^2)$. It enables one to interpret $\tau = [E_p^{(0)}\Omega \coth(\frac{1}{2}\beta\Omega)]^{-1/2}$ as the average time of phonon emission. This is a non-perturbative result that is valid for any model parameters. Finally, the sum rules may be employed to improve approximate analytic expressions for polaron spectral functions. Consider the two functions ($\mu = 0$, $T = 0$):

$$A_+^{\text{low}}(\mathbf{k}, \omega) = (2\pi)e^{-g_0^2} \sum_{m=0}^{\infty} \frac{g_0^{2m}}{m!} \times \delta(\omega + g_0^2\Omega - e^{-g_0^2}\varepsilon_{\mathbf{k}} - m\Omega), \quad (21)$$

$$A_+^{\text{high}}(\mathbf{k}, \omega) = (2\pi)e^{-g_0^2} \sum_{m=0}^{\infty} \frac{g_0^{2m}}{m!} \times \delta(\omega + g_0^2\Omega - \varepsilon_{\mathbf{k}} - m\Omega). \quad (22)$$

The first function is the one-polaron limit of Alexandrov and Ranninger's result for the Holstein model in the Lang-Firsov approximation [11]. In Eq.(21), $g_0^2\Omega$ is the zero-order binding energy $E_p^{(0)}$. A_+^{low} correctly describes the low-energy physics of the polaron, most notably the polaron band narrowing. However, it satisfies neither of the sum rules except the zeroth one. In particular, the first moment is equal to $e^{-g_0^2}\varepsilon_{\mathbf{k}}$ instead of the correct $\varepsilon_{\mathbf{k}}$. The second function A_+^{high} is a "wild guess". It *does* satisfy the first and second moments (but not the third and fourth ones) but does not describe the band narrowing. A_+^{high} is wrong at low energies but may be accurate at high energies. This conjecture is supported by the anticipation that at high energies the electron should become "free" from phonons. Thus a good spectral function could be the one that interpolates from A_+^{low} at low energies to A_+^{high} at high energies. With reasonable parameterization, the interpolation parameters could also be deduced from the sum rules.

In conclusion, a series of sum rules on the polaron spectral function have been derived. The sum rules are valid in the low-density limit. The first moment has been generalized to finite density. A connection with the angle-resolved inverse photoemission spectroscopy has been established. The spectrum should display a gap which size correlates with the mean square deviation of the spectral function. Several other applications have been identified.

The sum rules are open to further generalizations to dispersive phonons and more complex interactions.

I am grateful to A. M. Bratkovsky, D. Stewart, J. E. Hirsch, and especially to A. S. Alexandrov for very useful discussions on the subject and critical reading of the manuscript.

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